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CPA Theory of the Magnetization in Rare Earth Transition Metal Alloys

by

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Abstract

Calculations were made of the magnetic moment per atom of the transition metal and the rare earth metal in the intermetallic compounds, $Gd_{1-x}Ni_x$, $Gd_{1-x}Fe_x$, $Gd_{1-x}Co_x$, and $Y_{1-x}Co_x$. A simple model of the disordered alloy consisting of spins localized on the rare earth atoms and interacting with a narrow d-band is considered. The magnetic moment of the alloy at zero temperature is calculated within the molecular field and Hartree-Fock approximations. Disorder is treated in the coherent potential approximation. Results are in good agreement with the experimental data obtained for the crystalline and amorphous intermetallic compounds. It is shown that the temperature dependence of the magnetic moments and Curie and ferrimagnetic compensation temperatures can be accounted for by a simple model assuming a RKKY interaction between the rare-earth moments and the transition metal pseudo spin. The interaction is mediated by an effective alloy medium calculated using the CPA theory and elliptic densities of states.

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CONTENTS

1. INTRODUCTION

The rare earth and the transition element alloys have been the subject of much interest because of the possibility of their use as excellent permanent magnets with high transition temperatures. The reviews by Taylor (1971), Burzo (1973), and Wallace (1973) demonstrate that numerous experimental investigations have been carried out on this subject. However, more detailed theoretical investigations have not to our knowledge been performed on these rather complicated systems.

The magnetic properties of the rare earth metals mainly result from the partially filled 4f shell. The magnetic 4f electrons are strongly localized and the magnetic moments of the rare earth ions are coupled to their neighbours by exchange interaction with the conduction band electrons. From energy-band calculations it follows that the conduction bands in hcp rare earth metals are similar to those of the 3d transition metals having the hcp structure. These bands are overlapping. Moreover, s-like and d-like bands are strongly hybridized (Harmon and Freeman 1974). Additionally, we know that at zero temperature the magnetization of pure iron-group transition metals is currently described in terms of itinerant 3d electrons. Because of the large magnetic moments of some of the rare earth metals and the considerably high Curie temperature of some of the iron-group metals, the rare earth - transition metal intermetallic compounds are very interesting magnetic materials.

The purpose of this report is to investigate to what extent the magnetic moments and the transition temperatures, can be understood. Because of the complexity of the systems, use will be made of very simple models. Although the alloys only exist in the form of stoichiometrically ordered compounds, we shall apply ideas from molecular field and coherent potential approximations. These theories disregard the effect of the positional ordering of the atoms. However, this should not impose any serious limitation, because the magnetic properties of $Gd_{1-x}Co_x$, for which there are several possible atomic arrangements, do not vary significantly (Burzo 1975); the same applies to YCo_5 (Krén 1969), fig. 1. We consider the Gd and Y compounds. The effect of the crystal field on the magnetic moment and the transition temperature of these compounds is small and can be neglected to a first approximation. In the second section of the temperature dependence of the moment is calculated on the basis of an effective Ruderman-Kittel-Kasuya-Yosida interaction (RKKY) using the pseudo spin ideas developed in a recent paper on pure transition metals by Liu (1976).

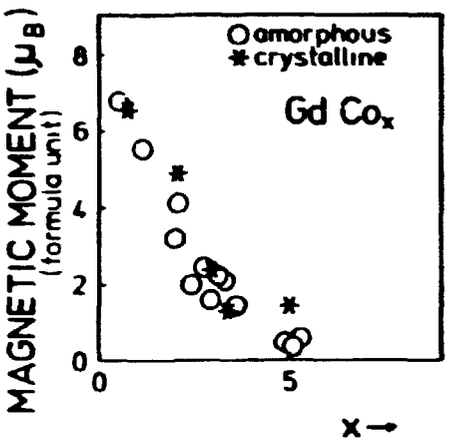

Fig. 1a. The composition dependence of the magnetic moment per formula unit for amorphous and crystalline Gd-Co_x compounds from Burzo (1975).

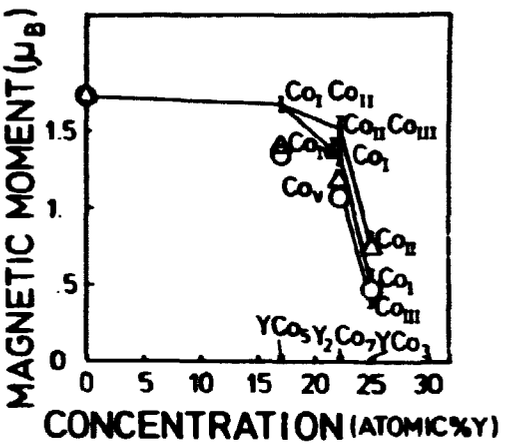

Fig. 1b. Magnetic moments associated with the different Co sites in pure Co, YCo_5, Y_2Co_7, YCo_3. The points connected by lines are from Krén (1969). Δ calculated mean value by the CPA theory, o mean values of data from Wallace (1973).

The third section gives a more detailed account of the polarization of the conduction electrons at the rare earth ions. Section four compares the theoretical and experimental results. Part of the presented results were recently published by Szpunar and Kozarzewski (1976) and Szpunar and Lindgård (1976).

2. SIMPLE THEORY OF THE TEMPERATURE DEPENDENCE OF THE MAGNETIC MOMENTS

The temperature dependence of the total magnetic moment for the rare earth intermetallic compounds has been found experimentally to be quite complex (Taylor 1971, Wallace 1973). The rare earth spin (R) and the 3d metal spin (T) order antiferromagnetically. The different magnitudes and temperature variations of the moments give rise to a ferrimagnetic compensation point, $T_{comp.}$, at which the total moment is cancelled. Buschow (1971) has propounded arguments for a qualitative understanding of the phenomena by using a free electron Fermi-momentum, k_F, as a parameter. Here we shall consider a more realistic, yet exceedingly simple model for the RT alloys. Liu (1976) has recently demonstrated that the temperature

dependent effects in itinerant magnets can well be accounted for by a quasi spin model. The quasi spins consist of highly correlated spin clouds around each T-atom. When excited, they are assumed to precess rigidly, and Liu showed that they interact mutally with an effective RKKY interaction. This model is clearly ideal for the RT alloys because we can now assume all interactions to be of the RKKY type mediated by the conduction electrons of the alloy.

The exchange Hamiltonian for the random alloy is then

$$H_{ex} = - \sum_{\substack{ij \\ ab}} p_i^a p_j^b J_{ij}^{ab} \vec{S}_i^a \cdot \vec{S}_j^b = - \frac{1}{N} \sum_q c_a c_b J^{ab}(q) \vec{S}_q^a \cdot \vec{S}_q^b \qquad (1)$$

where a and b indicate the type of atom, and the configurational average of the probabilities is equal to the concentrations, $p^a = c_a$ in the virtual crystal approximation. The Fourier transformed exchange integral is proportional to

$$J^{ab}(q) \propto \sum_k \frac{f_k(1-f_{k+q})}{\epsilon_k - \epsilon_{k+q}} \cdot j_a(k,k+q) j_b(k,k+q) \qquad (2)$$

where ϵ_k is the energy of the conduction electrons in the alloy, f_k the Fermi function, and $j^a_{k,k+q}$ the matrix element of the exchange interaction between the localized (quasi) spin of type a and the conduction electrons. Ferromagnetic ordering of any pair a-a is clearly obtained from (1) when $J^{aa}(q=0)$ is maximum. Assuming for simplicity, as is common, that $j^a_{k,k+q} = j_a$ is nearly independent of k and q we can write $J^{aa}(0)$ as

$$J^{aa}(0) \propto j_a^2 N_{alloy}(\epsilon_F) \qquad (3)$$

where $N_{alloy}(\epsilon_F)$ is a weighted average alloy density of states at the Fermi energy. Consistent with the random alloy theory, we then also assume that

$$J^{ab}(0) = j_a j_b N_{alloy}(\epsilon_F) \qquad a \neq b \qquad (4)$$

is maximum and negative when j_a and j_b have different signs. This gives antiferromagnetic ordering of all odd pairs a-b. To the same level of approximation we now consider the spin statistics of (1) in the molecular field approximation. One point must be clarified first. From the experimentally determined J(q) for Gd (Koehler et al. (1970)), it can be shown

that the self-energy $J_{ii} = \frac{1}{N}\sum_q J(q)$ is very small; assuming this to be generally true, we omit a subtraction of $\frac{1}{N}\sum_q J^{ab}(q)$ from (2). The molecular field acting on an atom of type a is then

$$H^a_{mol} = (c_a j_a \langle S^a_z \rangle + c_b j_b \langle S^b_z \rangle)\ j_a N_{alloy}(\varepsilon_F) \tag{5}$$

If the exchange interaction (1) is much stronger than the crystal field, the average magnetizations are given by the Brillouin function B_s:

$$\langle S^z_a \rangle = S_a B_{S_a}(H^a_{mol} S_a / kT) = \mathrm{Tr}\ S^z_a e^{-H^a_{mol} S^z_a / kT} / \mathrm{Tr}\ e^{-H^a_{mol} S^z_a} \tag{6}$$

where S_a is the maximum spin of the quasi spin of type a at T = 0. The advantage of using B_s, rather than the trace, is that non-integral values of the spin can easily be approximately taken into account. The total moment is

$$M_{total} = \sum_{n=a,b} g_n \mu_B c_n \langle S^z_n \rangle \tag{7}$$

The condition for the transition temperature for the present model was given by Lindgård (1975) in terms of the elemental paramagnetic susceptibilities

$$\left(\frac{1}{\chi^o_a(T)} - c_a J^{aa}(0)\right)\left(\frac{1}{\chi^o_b(T)} - c_b J^{bb}(0)\right) = c_a c_b (J^{ab}(0))^2 \tag{8}$$

This equation includes the anisotropy effect of the crystal field. However, for dominant exchange interaction, and using (3) and (4), we simply find

$$kT_c = \frac{1}{3} N_{alloy}(\varepsilon_F) \sum_{n=a,b} j_n^2 S_n(S_n+1) c_n \tag{9}$$

The deviation from a straight line interpolation between the transition temperatures for the pure elements are therefore mainly governed by $N_{alloy}(\varepsilon_F)$ in this model, and to a lesser extent by the variation of the quasi spin of T. For the compensation temperature we find, from (8), by expanding the Brillouin functions near T_c:

$$kT_{comp.} = \frac{1}{3} N_{alloy}(\varepsilon_F) \frac{X_1 X_2 c_1 c_2 j_1 j_2 (j_1 - j_2)\{(2X_2+1) j_2^2 - (2X_1+1) j_1^2\}}{(X_1(2X_1+1) c_1 j_1^3 + X_2(2X_2+1) c_2 j_2^3)}$$

where $X_i = S_i(S_i+1)$ (10)

The important quantities we need are the alloy density of states at the Fermi energy $N_{alloy}(\epsilon_F)$ and the polarization of the conduction electrons (at T=0), which constitutes the quasi spin for the 3d metal ion and the increase in moment for the rare earth ion. Using the coherent potential approximation (CPA), these quantities can be found at T = 0 and extensions made for higher temperatures. A comparison with the calculated and experimental temperature variations of the total as well as of the individual moments will be shown. The agreement is quite satisfactory. The values used for the parameters are given in table 2.

3. THE COHERENT POTENTIAL APPROXIMATION

3.1. Zero Temperature CPA Theory Neglecting Spin Flip Scattering

We consider a simple model consisting of spins localized on sites occupied by rare earth metal atoms and the narrow band formed essentially with 5d and 3d states from the rare earth and transition metals, respectively. The coupling between localized spins and band electrons for Gd is assumed to be the usual exchange interaction (Freeman 1973). Each lattice site is randomly occupied by a rare earth or transition metal atom with probabilities c_R and $c_T = 1 - c_R$, respectively. The corresponding Hamiltonian for s-d band electrons is assumed to have the form

$$H_{el} = H_d + H_{f-d}, \tag{11}$$

where

$$H_d = \sum_{iss'} (\epsilon_i - \tfrac{1}{2} g' \mu_B \mathcal{H} \sigma^z_{ss'}) c^+_{is} c_{is'} + \tfrac{1}{2} \sum_{is} U_i n_{is} n_{i-s} + \sum_{i \neq js} T_{ij} c^+_{is} c_{js} \tag{12}$$

is the form of non-degenerate narrow band Hubbard Hamiltonian in the external magnetic field $\mathcal{H}$,

$$H_{f-d} = - I \sum_{iss'} p_i S_i \sigma_{ss'} c^+_{is} c_{is'} \tag{13}$$

H_{f-d} is the exchange interaction of band electrons with localized spins, where $p_i = 1$ or 0, depending on whether the site at r_i is or is not occupied by a rare earth atom. Clearly, this model ignores 5-fold d-band degeneracy, which, however, can be qualitatively taken into account if U is thought of as

effective Coulomb repulsion and the calculated quantities, e.g. the average number of electrons, are multiplied by five. Also disorder is treated approximately in the transfer term T_{ij}:

$$T_{ij} = w_i t_{ij} w_j^* , \tag{14}$$

where the parameters w_i depend on the type of atom occupying the i'th site (they characterize the band width of pure metals) and t_{ij} is independent of configuration.

The known methods for dealing with disordered systems cannot be applied directly to the Hamiltonian (11). Therefore we have to introduce the Hartree-Fock approximation for intra-atomic Coulomb repulsion, which approximation has been widely used in transition metals alloys (Hasegawa and Kanamori 1972). At zero temperature, the spin fluctuation can be neglected and the term H_{f-d} is of simpler form

$$\tilde{H}_{f-d} = -I \sum_{is} p_i S_i^z \sigma_{ss}^z c_{is}^+ c_{is} . \tag{15}$$

Taking into account the experimental data for the compounds investigated (Taylor 1971), we assume the following values:

$$\text{for Y:} \quad S_i^z = 0 \tag{16}$$

$$\text{for Gd:} \quad S_i^z = S \cdot \mathrm{sgn}(M_i) . \tag{17}$$

In (17) we take advantage of the fact that the exchange coupling between the localized spins and the band electrons for Gd is positive. M_i is the magnetic moment of the conduction band electrons of Gd.

Making use of this assumption the Hamiltonian[1] H_{el} is replaced by $\tilde{H}_{el}$ where

$$\tilde{H}_{el} = \sum_{is} \epsilon_{is} n_{is} + \sum_{i \neq j s} T_{ij} c_{is}^+ c_{js} , \tag{18}$$

$$\epsilon_{is} = \epsilon_i + U_i \langle n_{i-s} \rangle - (\tfrac{1}{2} g' \mu_B \mathcal{H} + I p_i S_i^z) \sigma_{ss}^z . \tag{19}$$

In order to find the configuration of the averaged magnetic moments for both kinds of atom, we do as follows:

It is assumed that ϵ_{is} will be self-consistently determined in such a way that it only depends on the type of atom occupying the i'th site. This means now that

$$\langle n_{is} \rangle = \begin{cases} \langle n_{Rs} \rangle & \text{for rare earth sites} \\ \langle n_{Ts} \rangle & \text{for transition metal sites.} \end{cases}$$

We apply the locator formalism of the single site CPA (Shiba 1971) to find local densities of states of both rare earth and transition metal atoms.

Following Shiba (1971), let us introduce the bare locator

$$L_{is}(\omega) = \frac{\omega - \epsilon_{is}}{|w_i|^2}, \tag{20}$$

where i = R or T depending on whether site i is occupied by the rare earth or the transition metal atom. We also introduce the coherent locator $\tilde{L}_s(\omega)$. In this formalism the CPA equation for $\tilde{L}_s(\omega)$ has the following form:

$$c_R(L_{Rs}(\omega) - J_s(\omega))^{-1} + c_T(L_{Ts}(\omega) - J_s(\omega))^{-1} = F_s(\omega) \tag{21}$$

where

$$J_s(\omega) = \tilde{L}_s(\omega) - F_s^{-1}(\omega),$$

$$F_s(\omega) = \frac{1}{N} \sum_{\underline{k}} \frac{1}{\tilde{L}_s(\omega) - \epsilon_{\underline{k}}} = \int_{-\infty}^{\infty} \frac{N(\epsilon)\,d\epsilon}{\tilde{L}_s(\omega) - \epsilon} \tag{22}$$

and $\epsilon_{\underline{k}}$ is defined through

$$t_{ij} = \frac{1}{N} \sum_{\underline{k}} \epsilon_{\underline{k}}\, e^{-i\underline{k}(\underline{r}_i - \underline{r}_j)}.$$

The main quantities that we are looking for are local (or partial) densities of states of the rare earth and the transition metal atoms

$$\rho_{is}(\omega) = -\frac{1}{\pi |w_i|^2} \operatorname{Im} \frac{1}{\tilde{L}_{is}(\omega) - J_s(\omega)}. \tag{23}$$

The Gd and Y compounds considered here have various and quite complicated crystallographic structures (Cromer and Larson 1959).

For ease of computation we use the simple analytic form of the density of states

$$N(\omega) = \begin{cases} \frac{2}{\pi}\sqrt{1-\omega^2} & \text{for } |\omega| \leq 1 \\ 0 & \text{otherwise .} \end{cases} \tag{24}$$

This assumption means that the half bandwidth of the pure transition or rare earth metal is given by $|w_T|^2$ or $|w_R|^2$, respectively. Then, $J_s(\omega) = F_s(\omega)/4$ and the CPA equation (21) is replaced by

$$c_R(L_{Rs}(\omega) - \tfrac{1}{4}F_s(\omega))^{-1} + c_T(L_{Ts}(\omega) - \tfrac{1}{4}F_s(\omega))^{-1} = F_s(\omega) \tag{25}$$

and

$$\begin{aligned} n_{is} &= \int_{-\infty}^{\epsilon_F} \rho_{is}(\omega)\,d\omega \\ &= -\frac{1}{\pi|w_i|^2}\int_{-\infty}^{\epsilon_F} \mathrm{Im}\,\frac{1}{\omega-\epsilon_{is}-\frac{1}{4}F_s(\omega)}\,d\omega\ , \end{aligned} \tag{26}$$

where ϵ_F is the Fermi energy obtained self-consistently from the given number of electrons in the compounds N:

$$N = c_R N_R + c_T N_T\ . \tag{27}$$

where N_R and N_T are the numbers of electrons per one atom in the pure rare earth metal and in the transition metal, respectively. The expectation values for the number of electrons with spins in R and T sites are determined by solving self-consistency conditions (19) and (26) and eq. (25).

In this way, both the band electrons (including 5-fold degeneracy of the d-band) and the localized spin contribute to the magnetic moment. For the transition metal atom, this contribution is

$$M_T = \frac{5}{2}g'\mu_B(n_{T\uparrow} - n_{T\downarrow})\ . \tag{28}$$

Similarly, the contribution from the rare earth atom is:

$$M_R = g\mu_B S^z + \frac{5}{2}g'\mu_B(n_{R\uparrow} - n_{R\downarrow})\ . \tag{29}$$

The total magnetic moment per atom of an alloy is:

$$M = c_T M_T + c_R M_R\ . \tag{30}$$

3.2. Temperature Dependence of the Rare Earth Conduction Electron Polarization Including Spin Flip Scattering

Using the CPA results at T = 0, it was in section 2 demonstrated that a good qualitative description of the temperature dependence of the magnetization can be obtained by assuming a Ruderman Kittel interaction between the localized 4f spins of the rare earth ions and the quasi spins (Liu 1976) of the transition metal ions. In this model we neglected the conduction electron polarization of the rare earth ions. The simplest way to include this effect is to assume a polarization proportional to the average rare earth moment, $M_R(T)$. However, let us here calculate this effect with the CPA theory. Whereas the polarization at zero temperature is well given by the usual CPA theory, which neglects spin flip scattering (Szpunar, Kozarzewski 1976), it is essential to include this effect in order to calculate the temperature dependence (Liu 1976). In the rare-earth-rich compounds the polarization of the rare earth conduction electrons is large, but the transition metal quasi spin is small and can be neglected.

The interaction between the localized 4f electrons and the band electrons is now given by

$$H_{fd} = - I \sum_{i,\sigma\sigma',\alpha} \delta_{i,R} S_i^{\alpha} \sigma^{\alpha}_{\sigma\sigma'} c^{+}_{i\sigma} c_{i\sigma'} \qquad (31)$$

where σ^{α} is the Pauli matrixes, S the localized spin and I the exchange interaction. Kubo (1973) developed a CPA theory for the effect of the scattering (including spin flip) of electrons on localized spins in magnetic semiconductors. Here we shall closely follow this approach and generalize it to cover the rare earth transition metal case. Neglecting the quasi spin of the transition metal ions and considering only the localized rare earth spins (for the rare earth rich alloys), we can write the elements of the locator (Shiba 1971, Kubo 1973) at the origin for the Hamiltonian (11) for an electron with spin up

$$\begin{aligned}
(L_o)_{\uparrow\uparrow} &= \frac{1}{|w_o|^2}\{\omega - H^{\uparrow}_{o,d} + IS_o^z\} \\
(L_o)_{\downarrow\downarrow} &= \frac{1}{|w_o|^2}\{\omega - H^{\downarrow}_{o,d} + \delta_{o,R}\,[H_{Mol} - I(S_o^z + 1)]\} \\
(L_o)_{\uparrow\downarrow} &= (L_o)_{\downarrow\uparrow} = \delta_{o,R}\,\frac{I}{|w_o|^2}\sqrt{(S - S_o^z)(S + 1 + S_o^z)}
\end{aligned} \qquad (32)$$

Similarly for an electron with spin down

$$(L_o)^{\downarrow\downarrow} = \frac{1}{|w_o|^2}\{\omega - H^{\downarrow}_{o,d} - IS^z_o\}$$

$$(L_o)^{\uparrow\uparrow} = \frac{1}{|w_o|^2}\{\omega - H^{\uparrow}_{o,d} - \delta_{o,R}\,[H_{Mol} - I(S^z_o - 1)]\} \qquad (33)$$

$$(L_o)^{\uparrow\downarrow} = (L_o)^{\downarrow\uparrow} = \delta_{o,R}\,\frac{I}{|w_o|^2}\sqrt{(S+S^z_o)(S+1-S^z_o)}$$

where:

$$H^{\sigma}_{i,d} = \varepsilon_i + U_i\langle n_{i,-\sigma}\rangle - \alpha_{\sigma}\frac{1}{2}g_s\mu_B H_{ext}, \quad \alpha_{\uparrow} = 1, \quad \alpha_{\downarrow} = -1 \qquad (34)$$

H_{Mol} is the molecular field, as defined in the previous section (5), experienced by the rare earth localized spin. The energy H_{Mol} is transferred to or absorbed from the spin flip scattering electron when the localized spin changes its spin projection S^z_o by one unit. In (32) we consider for example, the localized initial state to be $|S, S^0_z\rangle$ and have expressed $\langle S, S^z_0 + 1 \,|\, S^+ \,|\, S, S^z_0\rangle$ in the operator form $\sqrt{(S-S^z_0)(S+1+S^z_0)}$. We can now write the CPA equation

$$\langle x(L_A - J)^{-1} + (1-x)(L_B - J)^{-1}\rangle = F \qquad (35)$$

where $J^{\sigma} = \tilde{L}^{\sigma} - 1/F^{\sigma}$ and

$$F^{\sigma} = \frac{1}{N}\sum_k (\tilde{L}^{\sigma} - \varepsilon_k)^{-1} = \int_{-\infty}^{\infty} \frac{N(\varepsilon)}{\tilde{L}^{\sigma} - \varepsilon}\, d\varepsilon \qquad (36)$$

is the propagator for the effective medium, $\tilde{L}^{\sigma}$ is the coherent locator. For the elliptic density of states (24), one finds (Szpunar and Kozarzewski 1976) that $F^{\sigma} = 4J^{\sigma}$. $\langle \ldots \rangle$ denotes the thermal average

$$\langle A\rangle = \mathrm{Tr}\, A\, e^{-\beta H_{Mol} S^z} / \mathrm{Tr}\, e^{-\beta H_{Mol} S^z}, \quad \beta = \frac{1}{kT} \qquad (37)$$

However, in order to simplify the calculations, we simply replace S^z by $\langle S^z\rangle$ in the various expressions; an approximation that is valid at low temperatures. The CPA equation (35) can now be solved by multiplying by $(L_A - J)$ and $(L_B - J)$ to give $(L_i)^{\sigma\sigma'} \approx 0$ for i = Co, Ni, Fe, $\sigma \neq \sigma'$).

$$(J^\sigma)^3 - (J^\sigma)^2 (L_A^\sigma + L_B^\sigma) + J^\sigma (L_A^\sigma L_B^\sigma + \tfrac{1}{4}) - \tfrac{1}{4}(xL_B^\sigma + (1-x)L_A^\sigma) = 0 \quad (38)$$

From the analytic solution for J we can find the partial density of states (Shiba 1971)

$$\rho_i(\omega) = -\frac{1}{\pi}\frac{1}{|w_i|^2}\mathrm{Im}\left(\frac{1}{L_i - J}\right)^{\sigma\sigma} \quad (39)$$

Explicitly, this gives

$$\rho_R^\sigma(\omega) = -\frac{1}{\pi}\frac{1}{|w_R|^2}\mathrm{Im}\frac{A_\sigma}{A_\sigma B_\sigma - C_\sigma^2} \quad (40)$$

where

$$A_\sigma = \frac{1}{|w_R|^2}\{\omega - H_{o,d}^{-\sigma} + \alpha_\sigma[H_{Mol} - I(\langle S^z\rangle + \alpha_\sigma)]\} - J^{-\sigma}$$

$$B_\sigma = \frac{1}{|w_R|^2}\{\omega - H_{o,d}^{\sigma} + \alpha_o I\langle S^z\rangle\} - J^{\sigma} \quad (41)$$

$$C_\sigma = \left(\frac{I}{|w_R|^2}\right)^2 (S - \alpha_\sigma\langle S^z\rangle)(S + 1 + \alpha_\sigma\langle S^z\rangle)$$

When the spin flip scattering term, C_σ, is neglected, the density of states (40) reduces to the result used at zero temperature for the calculation of the saturation moments (Szpunar and Kozarzewski, 1976). It is clear that C_σ is small when $\langle S^z\rangle \sim S$, but is significant at high temperatures when $\langle S^z\rangle \sim 0$, in accordance with the discussion by Liu (1976). The total density of states is $\rho(\omega) = x\rho_R(\omega) + (1 - x)\rho_T(\omega) \sim N_{alloy}(\omega)$. The conduction electron polarization of the rare earth metal ions is given by

$$M_i(T) = \frac{5}{2}g\mu_B \int_{-\infty}^{\infty} f(\omega)(\rho_i^\uparrow(\omega) - \rho_i^\downarrow(\omega))\, d\omega \quad (42)$$

where $f(\omega) = (e^{\beta(\omega - \epsilon_F)} + 1)^{-1}$ is the Fermi distribution function. The Fermi energy ϵ_F is determined by the condition that the total number of electrons, N, is conserved

$$N = xN_R + (1 - x)N_T, \quad (43)$$

where N_R and N_T are the number of electrons per atom of the pure rare earth and transition metal elements. The present model can in a straightforward way be generalized to include the effect of a quasi spin on the transition metal ion.

4. NUMERICAL RESULTS AND DISCUSSION

4.1. Zero Temperature Results

Here follows a comparison of the magnetic moments resulting from the presented model with the experimental data for the intermetallic compounds $Gd_{1-x}Ni_x$, $Gd_{1-x}Fe_x$, $Gd_{1-x}Co_x$, and $Y_{1-x}Co_x$. The model gives the antiferromagnetic ordering in all the compounds considered. Figs. 2a and 3 presents examples of the density of states in $Gd_{1-x}Co_x$ and $Gd_{1-x}Ni_x$ compounds calculated for antiferromagnetic ordering in the given model. The antiferromagnetic ordering is due to the difference between the integrated density of states of spin up and down electrons. Fig. 2b shows for comparison the paramagnetic density of states for $Gd_{1-x}Co_x$.

This antiferromagnetic ordering does not depend on the difference between the energy level of the rare earth metal atom and the transition metal atom in the compounds, or on the neighbouring mean surroundings of the atom. Neither does the calculated antiferromagnetism depend on the concentration of electrons in the compounds. This is in agreement with experimental results (Barbara 1973, Krén 1969).

In the case of the Ni compounds the calculated magnetic moment of Ni is small but antiparallel to the magnetic moment of Gd. The experimentally reported ferromagnetism for some of these compounds (Wallace 1973) is probably due to the big polarization of conduction bands of Gadolinium (table 1). A number of detailed results are given in table 1. Fig. 4 shows the total and the transition metal moment at zero temperature.

The theoretical approach presented is only based on parameters describing the electron structure of the pure metal: the integral of the Coulomb intra-atomic repulsion (U_i), the half bandwidth ($|w_i|^2$), the energy level (ϵ_i), the integral of exchange interaction between the localized spin of 4f electrons and the conduction band electrons (I), and the total number of electrons per atom. The intra-atomic Coulomb repulsion and the bandwidth for the pure metal were fitted to obtain the best agreement with the experimental value of the density of states at Fermi energy, and with the magnetic moment per one atom of the pure metal.

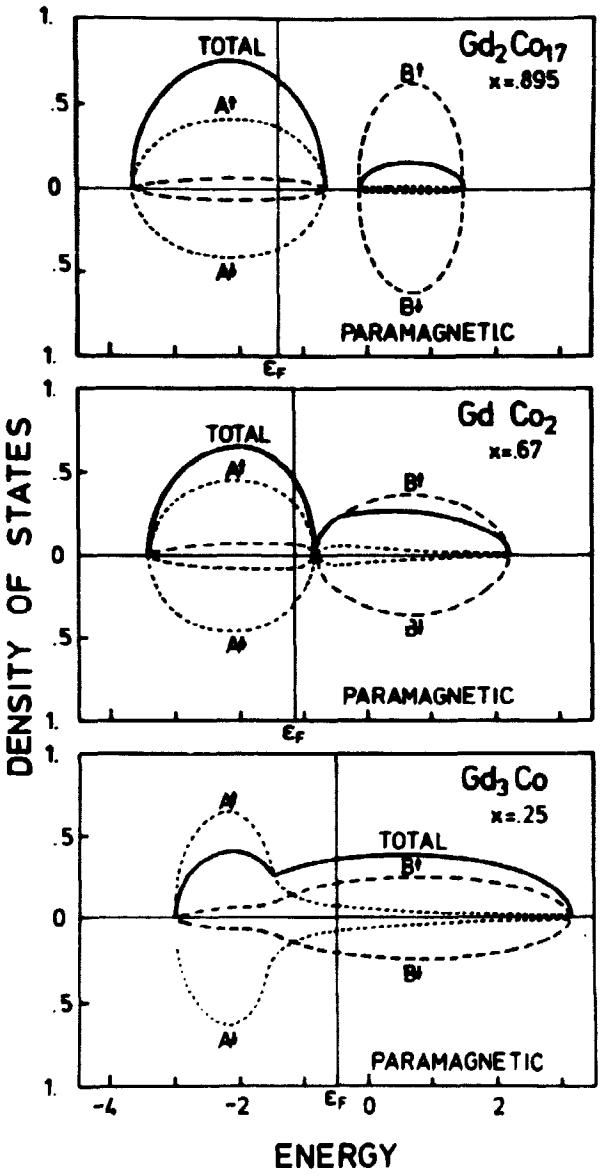

Fig. 2a. Density of states in Gd-Co compounds for paramagnetic ordering calculated from CPA theory. _____ $\rho(\varepsilon)_{total}$ ····· $\rho(\varepsilon)_{transition\ metal}$ ------ $\rho(\varepsilon)_{rare\ earth}$.

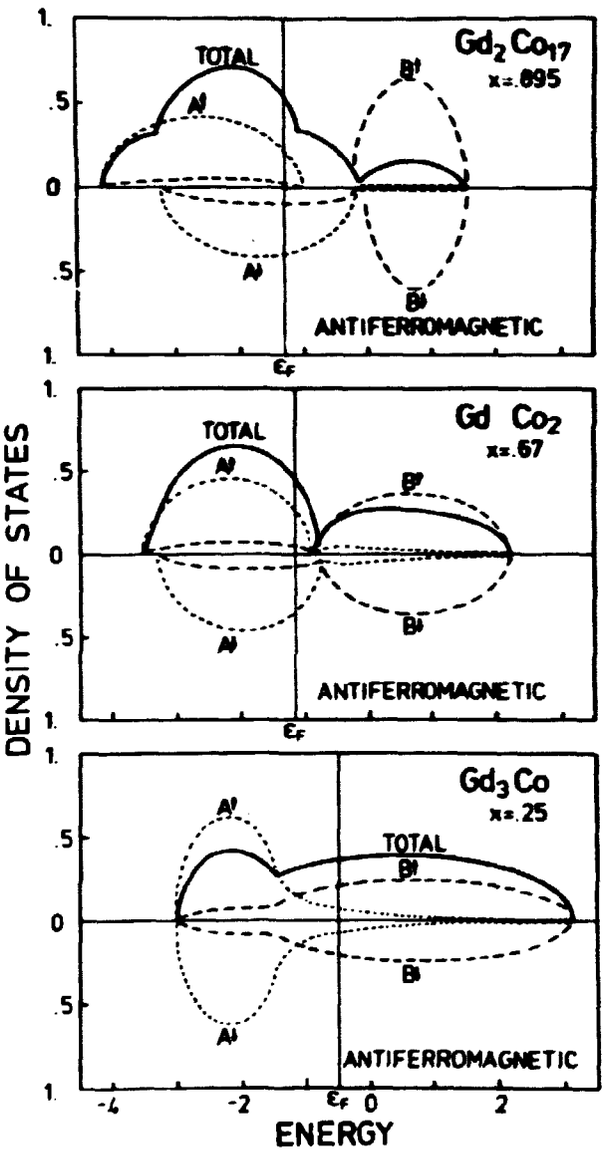

Fig. 2b. Density of states in Gd-Co compounds for antiferromagnetic ordering calculated from CPA theory. _____ $\rho(\epsilon)_{total}$ ····· $\rho(\epsilon)_{transition\ metal}$ ----- $\rho(\epsilon)_{rare\ earth}$.

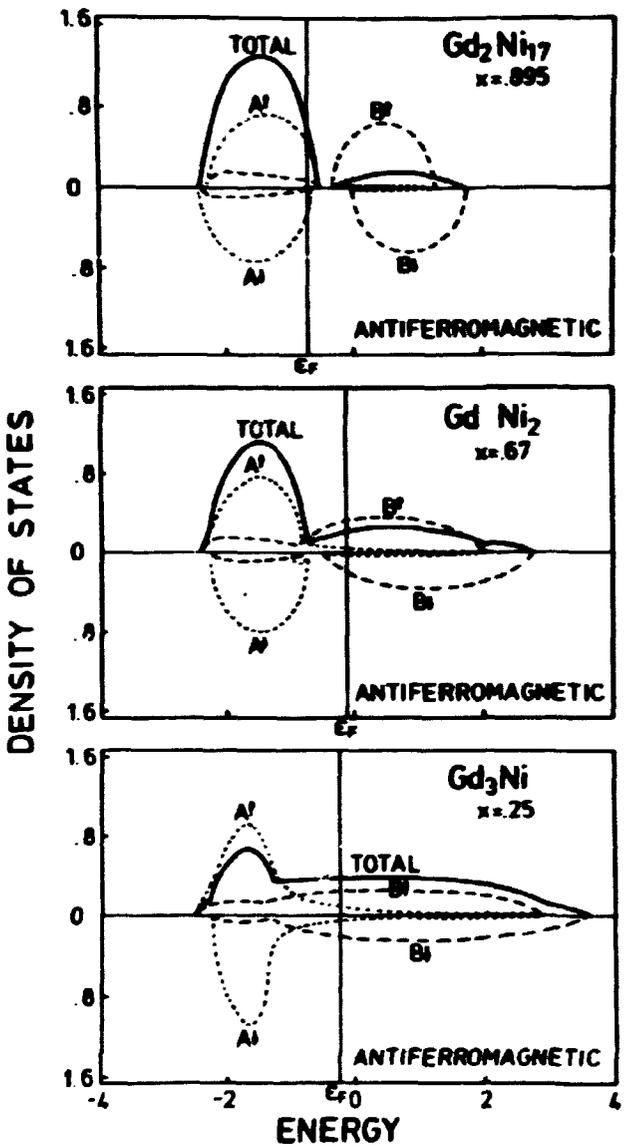

Fig. 3. Density of states in Gd-Ni compounds for antiferromagnetic ordering calculated from CPA theory. _____ $\rho(\varepsilon)_{total}$ ····· $\rho(\varepsilon)_{transition\ metal}$ ----- $\rho(\varepsilon)_{rare\ earth}$.

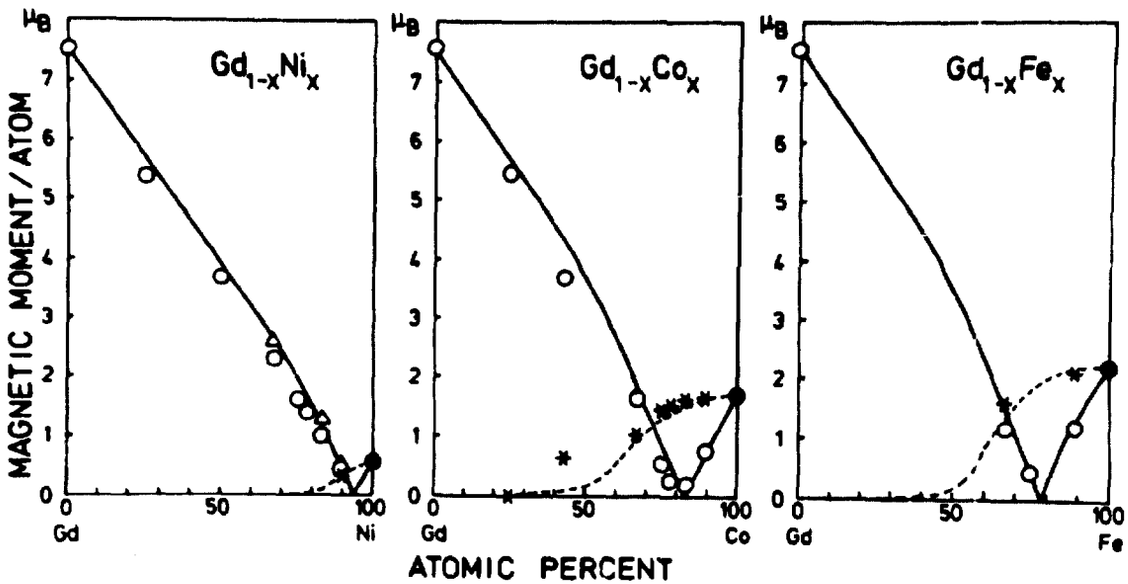

Fig. 4. Magnetic moment as function of concentration in Gd-Ni, Gd-Co, Gd-Fe compounds.
_____ average magnetic moment per atom ----- magnetic moment of transition metal atoms. Experimental points are taken from: Taylor (1971)(O), Burzo (1973)(Δ), Wallace (1973)(*), Burzo (1975)(*).

x	$R_{1-x}T_x$ compound	M_T (μ_B)	M_R (μ_B)	M^{theor} (μ_B)	M^{exp} (μ_B)	$\rho_{AFM}(\epsilon_F)$ (/atom eV)	$\rho_{PM}(\epsilon_F)$ (/atom eV)
1.	Ni	.6		.6	.6	2.7	4.4
.895	Gd_2Ni_{17}	-.3	7.4	.51	.46,.49	2.6	3.2
.83	$Gd\ Ni_5$	-.075	7.43	1.2	1.,1.13	.3	.45
.778	Gd_2Ni_7	-.04	8.03	1.75	1.4	.59	.9
.75	$Gd\ Ni_3$	-.03	8.18	2.02	1.63	.87	1.
.67	$Gd\ Ni_2$	-.01	8.17	2.69	2.33,2.37	1.19	1.3
.5	Gd Ni	-.01	7.91	3.95	3.7	1.53	1.6
.25	Gd_3Ni	-.01	7.68	5.76	5.4	1.83	1.85
.0	Gd		7.56	7.56	7.55	2.	2.
1.	Fe	2.2		2.2	2.2	3.29	3.75
.895	Gd_2Fe_{17}	2.2	-7.11	1.26	1.2	2.87	3.47
.79	Gd_6Fe_{23}	-1.97	-7.14	.05	?	2.52	3.13
.75	$Gd\ Fe_3$	-1.8	7.15	.43	.46	2.39	2.98
.67	$Gd\ Fe_2$	-1.36	7.17	1.46	1.25	2.2	2.65
.0	Gd		7.56	7.56	7.55	2.	2.
1.	Co	1.7		1.7	1.7	3.22	3.57
.895	Gd_2Co_{17}	1.65	-7.34	.71	.76	2.84	3.28
.83	$Gd\ Co_5$	1.52	-7.37	.01	.2	2.61	3.06
.778	Gd_2Co_7	-1.36	7.39	.57	.27	2.43	2.87
.75	$Gd\ Co_3$	-1.29	7.39	.88	.55	2.33	2.74
.67	$Gd\ Co_2$	- .93	7.42	1.83	1.65	2.03	2.34
.43	Gd_4Co_3	- .1	7.65	4.32	3.71	1.5	1.53
.25	Gd_3Co	- .05	7.63	5.7	5.48	1.77	1.79
.0	Gd		7.56	7.56	7.55	2.	2.
1.	Co	1.7		1.7	1.7	3.22	3.57
.895	$Y_2\ Co_{17}$	1.6	- .15	1.41	1.46	2.87	3.28
.83	$Y\ Co_5$	1.4	- .15	1.14	1.13	2.67	3.06
.778	$Y_2\ Co_7$	1.2	- .15	.88	.82	2.54	2.87
.75	$Y\ Co_3$	1.	- .14	.75	.35	2.47	2.74
.67	$Y\ Co_2$	.3	- .06	.21	?	2.28	2.34
.43	$Y_4\ Co_3$	.0	.0	.0	.02	1.53	1.53
.25	$Y_3\ Co$	.0	.0	.0	.25	1.79	1.79
.0	Y		.0	.0	.0	2.	2.

Table 1. Results of calculation. The magnetic moment is expressed in the Bohr magneton.

x - concentration of transition metal

M_T - average magnetic moment of transition metal atoms in compounds

M_R - average magnetic moment of rare earth metal atoms in compounds

M^{teor}, M^{exp} - magnetic moment per atom compounds

$\rho_{AFM}(\epsilon_F)$ - density of states at Fermi energy for antiferromagnetic solution

$\rho_{PM}(\epsilon_F)$ density of states at fermi energy for paramagnetic solution.

To calculate the interaction between the localized spin and the s-d band electron, I in Gadolinium, use was made of the following formula derived from molecular field theory (Lindgård 1974) and (9)

$$kT_c = \frac{1}{3}(g-1)^2 I^2 \rho(\epsilon_F) J(J+1) . \qquad (44)$$

The experimental value of Curie temperature T_c is used in this formula. The intra-atomic Coulomb repulsion for Gd, U_{Gd}, must be different from zero in order to give satisfactory values for the magnetic moment, the density of states at the Fermi energy, and the Curie temperature. This is in accordance with the predominant d-character of the band electrons, near the Fermi surface of Gadolinium (Harmon and Freeman 1974). The parameters of the model (table 2) are in good agreement with those proposed by other authors. For example, the intra-atomic Coulomb repulsion calculated by Cox et al. (1973) is for Co, Fe, Ni respectively equal to 3 eV, 2.7 eV, 3.3 eV. The exchange interaction between localized spins and conduction band electrons proposed by Freeman (1974) is .087 eV, by Gomes and Guimaraes (1974): .025 eV.

Metal	ε (eV)	$\|w\|^2$ (eV)	U (eV)	N (el/atom)	g'	g	S	I (eV)
Gd	0.0	3.0	1.9	3.0	2	2	3.5	.049
Y	0.0	3.0	1.9	3.0	2		0	
Co	-4.4	1.6	2.9	7.7	2			
Fe	-5.0	1.6	2.8	7.1	2			
Ni	-4.0	.9	2.7	9.4	2			

Table 2. Parameters of the model. The energy units used are electron volt.

ε - atomic energy level

$|w|^2$ - half bandwidth

U - intra-atomic Coulomb repulsion

N - number of electrons per atom in pure metal

g' - Lande factor of the conduction band electrons

g - Lande factor of the localized 4f electrons

S - localized spin of 4f electrons

I - exchange integral between localized spin and conduction band.

For $Y_{1-x}Co_x$ compounds, the same parameters are used as for $Gd_{1-x}Co_x$, only the localized spin of Y is equal to zero (table 1). Comparing the calculated values of the magnetic moment per atom of rare earth metal and of transition metal given in table 2 with the experimental data (Taylor (1971), Burzo (1973), Wallace (1973), Krén (1969)), we can conclude that the presented simple model for disordered alloys gives relatively good values for the magnetic moment in all the intermetallic compounds considered. The calculated magnetic moment of the transition metal decreases as the concentration of Gadolinium increases. The magnetic moment of Co in $Y_{1-x}Co_x$ compounds is smaller than in the corresponding $Gd_{1-x}Co_x$ compounds. This also agrees with experiment (Wallace 1973, Taylor 1971, Burzo 1973), fig. 5. Our model calculations are in accordance with the experimental fact (Figiel et al. 1976) that the magnetic moment of Yttrium in Y_2Co_{17}, YCo_5, Y_2Co_7 and YCo_3 compounds seems not to be related to the magnitude of the magnetic moment of the Co atoms (table 1).

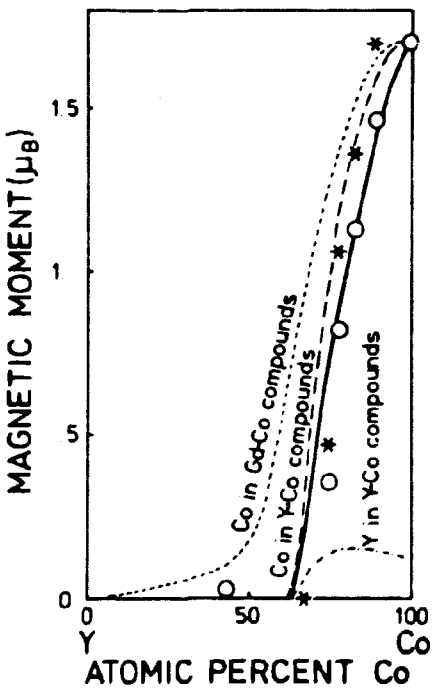

Fig. 5. Magnetic moment as function of concentration in Y-Co and Gd-Co compounds. _____ average magnetic moment per atom of compounds, ----- average magnetic moment of Co atoms in Y-Co compounds, ... magnetic moment of Co atoms in Gd-Co compounds, -·-·-· magnetic moment of Y atoms in Y-Co compounds. Experimental points are taken from: Taylor (1971) (O), Wallace (1973) (*).

The assumption of the simple elliptic density of states was satisfactory for the calculation of magnetization in the whole interval of concentration of Gadolinium and Yttrium. This is easy to understand because the magnetic moment is calculated from the integral of the density of states, thus the shape of the density is not particularily important.

We have demonstrated that the proposed CPA model gives good semi-quantitative agreement with a considerable amount of experimental data. Although simple the theory is presumably more realistic than the current arguments (Buschow 1971) using the Fermi momentum k_F as a parameter and other phenomenological models (Eagles 1973, Gomes and Guimaraes 1974).

4.2. Finite Temperature Results

The good agreement between the calculated and measured Curie temperatures for the $Gd_{1-x}Co_x$ alloys, fig. 6, demonstrates that the simple model of an effective RKKY interaction between the Gd-localized spin and the Co-pseudo spin works very well. The same is the case for the $Y_{1-x}Co_x$ alloys using the same parameters. The two exchange parameters for the pure elements have been chosen to fit (table 3). The relation between the exchange constants follows from (3) and (4)

$$J^{ab}(0)^2 = J^{aa}(0)\,J^{bb}(0)$$

Metal	Gd	Y	Co	Fe	Ni
$\lvert j^{AFM}\rvert$ (eV)	.049	-	.267	.188	.392
$\lvert j^{PM}\rvert$ (eV)	.049	-	.253	.176	.304

Table 3. Parameters of the Model. The exchange interaction between the localized (pseudo) spin and the conduction electrons in eV for the antiferromagnetic (AFM) and paramagnetic (PM) densities of states

This dependence was found from the experimental data for the $(Gd_xY_{1-x})Co_2$ compounds (x = 0.4 to 1) by Burzo (1975). Furthermore it was found that the rare earth metal susceptibility for these compounds is nearly constant. This is in agreement with our model because we expect the density of states at the Fermi energy to be essentially independent of the type of rare earth ion. For an alloy of two rare earth metals, the transition temperatures fall on a nearly straight line (Koehler 1972). The marked deviation from the straight line shows that the density of states in the $Gd_{1-x}Co_x$ alloy varies strongly with concentration; a variation which is well accounted for by the simple elliptic model densities of states used here. The agreement is also reasonable for $Gd_{1-x}Ni_x$ alloys. The reason is presumably that the exchange interactions (3 and 4) are proportional to a weighted average density of states $N_{alloy}(\epsilon_F)$ near the Fermi energy and that the symmetry of the lattice is very low, and therefore gives rise to a rather featureless density of states. However, the $Gd_{1-x}Fe_x$ alloys show marked deviations from the calculations based on the elliptic density of states. This is in fact not very surprising because it is known that the Fermi energy falls at a pronounced peak in the density of states for pure bcc Fe (Madsen et al. 1975). The structure of the alloys has low symmetry. Since the Fermi energy and the alloy density of states change with concentration, far more dramatic changes may be expected than can be obtained by the smooth elliptic density of states. A calculation using a more realistic density of states would be of interest. However, in this case it is of importance to take into account the changes in symmetry of the various alloys. Model calculations of the density of states for different structures of Fe show large differences in $\rho(\epsilon_F)$ (Madsen et al. 1975).

The calculated temperature dependence of the total magnetic moment is in semi-quantitative agreement with the observations for the $Gd_{1-x}Co_x$ alloys. Figs. 7 and 8. The temperature dependence of the Gd and Co moments is given on fig. 9. It is interesting that the simple molecular field theory combined with the CPA density of states correctly predicts a compensation point for the observed concentrations. At high temperature the paramagnetic density of states gives the best agreement, as to be expected. For the reasons given above the elliptic density of states is too crude an approximation to account for the detailed temperature behaviour in the $Gd_{1-x}Ni_x$ and $Gd_{1-x}Fe_x$ alloys. The results for the Ni alloys are shown on figs. 10, 11 and 12. The inclusion of the conduction electron polarization calculated by the CPA spin flip theory is in good agreement with observations for Gd, fig. 8. The polarization closely follows a simple

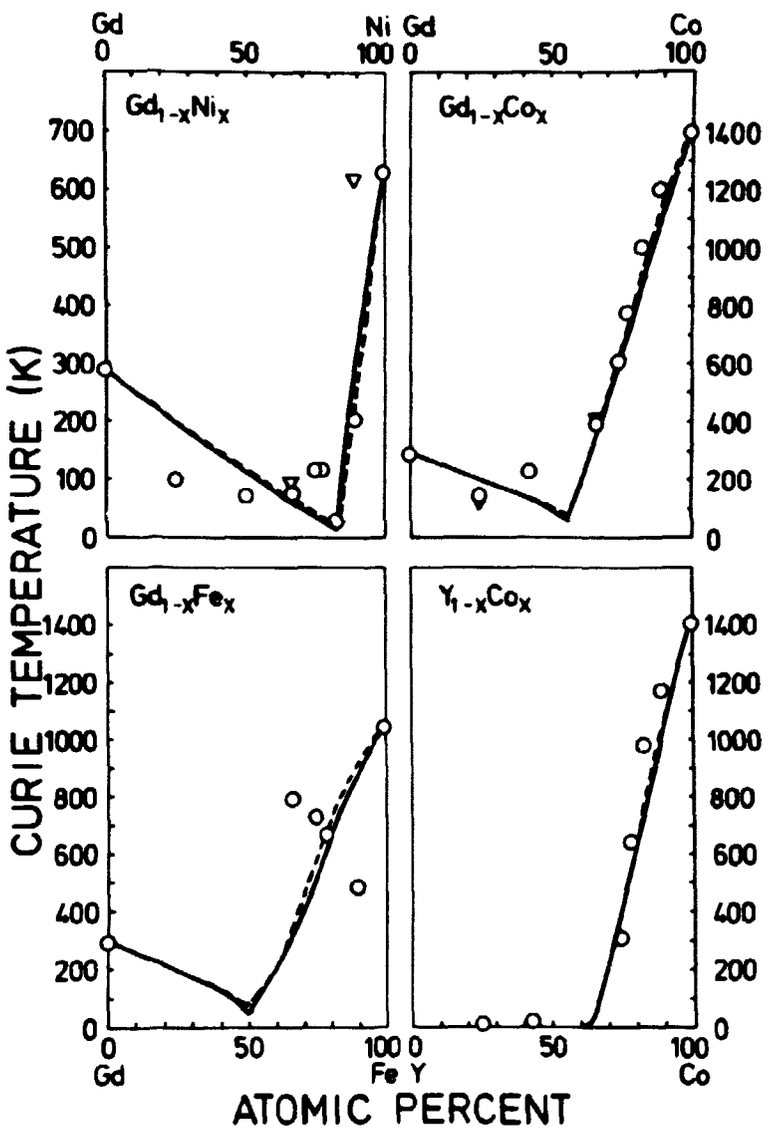

Fig. 6. Curie temperature as function of concentration of transition metal in: a) Gd-Ni compounds b) Gd-Co compounds c) Gd-Fe compounds d) Y-Co compounds. Experimental points are taken from papers Bozorth (1959) (O), Burzo (1973) (O), Taylor (1971) (O), Wallace (1973) (▽), Rhyne (1973) (O).

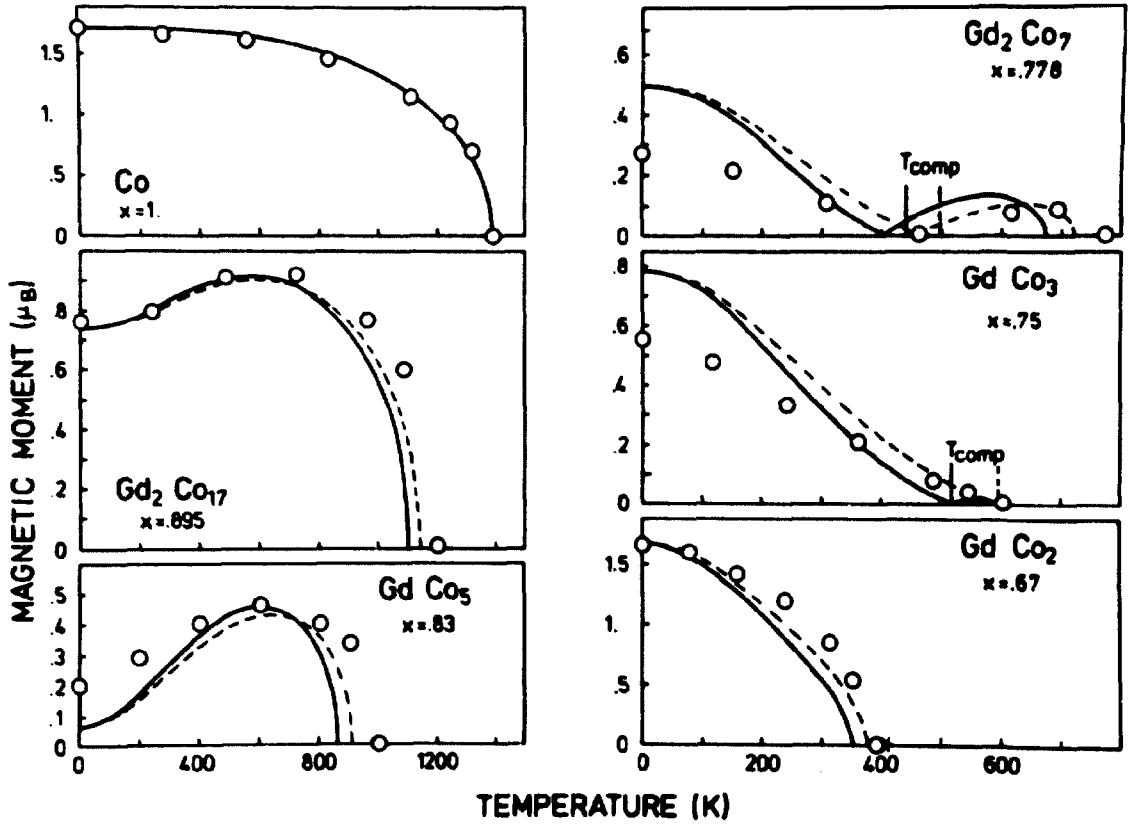

Fig. 7. Average magnetic moment atom in Gd-Co compounds as function of temperature calculated from molecular field theory. (___ AFMρ(ϵ_p) --- PMρ(ϵ_p)). Experimental points are taken from Burzo (1975) (O). Taylor (1971) (*).

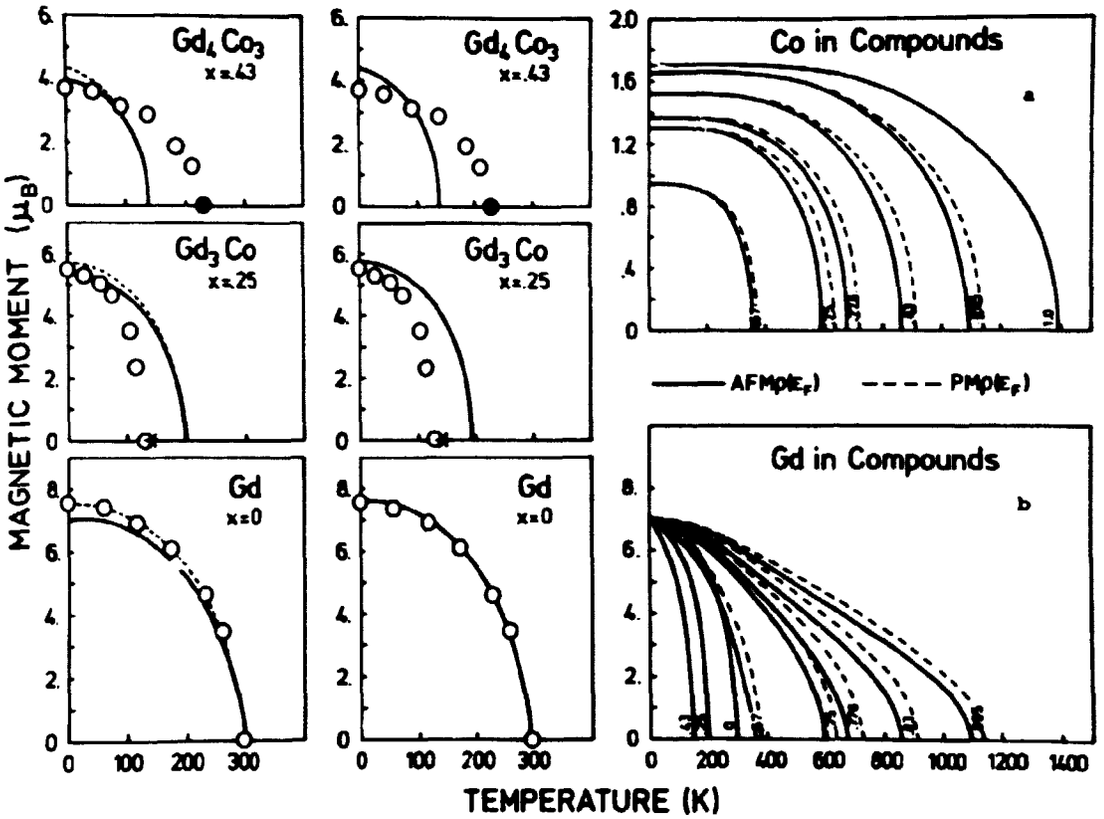

Fig. 8a. Fig. 8b. Fig. 9

Fig. 8a. Average magnetic moment per atom in Gd-Co compounds as function of temperature calculated from molecular field theory. (___ AFMρ(ε_F)---PMρ(ε_F)). Experimental points are taken from Burzo (1975)(O), Taylor (1971)(*).

Fig. 8b. CPA calculation of the average magnetic moment per atom in Gd-Co compounds as function of temperature (___AFMρ(ε_F) --- PMρ(ε_F)). Experimental points are taken from Burzo (1975)(O), Taylor (1971)(*).

Fig. 9a. Magnetic moment of Co in Co-Gd compounds as function of temperature calculated from molecular field theory.

Fig. 9b. Magnetic moment of Gd in Co-Gd compounds as function of temperature calculated from molecular field theory.

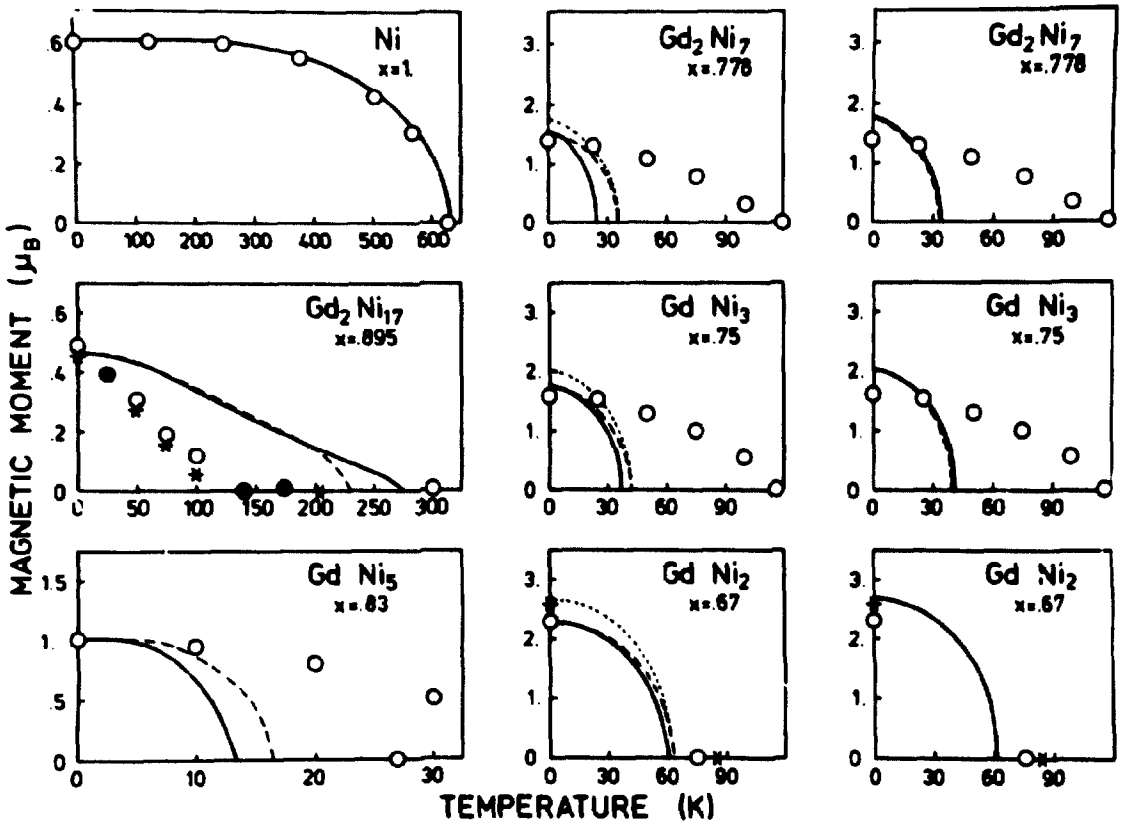

Fig. 10. Average magnetic moment per atom in Gd-Ni compounds as function of temperature calculated from molecular field theory. (___AFMρ(ε_F)--- PMρ(ε_F)). Experimental points are taken from: Kittel (1956)(□), Lemaire et al (1967)(○), Paccard et al (1967)(○), Taylor (1971)(•).

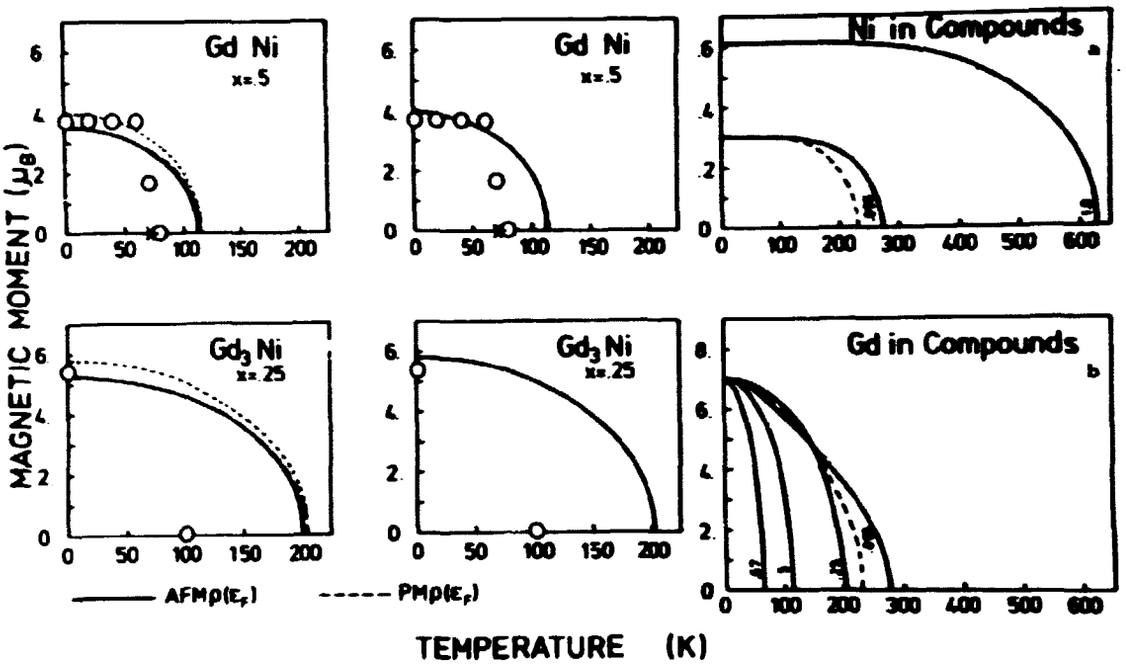

Fig. 11a. Fig. 11b. Fig. 12

Fig. 11a. Average magnetic moment per atom in Gd-Ni compounds as function of temperature calculated from molecular field theory. Experimental points are taken from Walline et al (1964)(O), Taylor (1971)(•).

Fig. 11b. CPA calculation of the average magnetic moment per atom in Gd-Ni compounds as function of temperature. Experimental points are taken from Walline et al (1964)(O), Taylor (1971)(•).

Fig. 12a. Magnetic moment of Ni in Ni-Gd compounds as function of temperature calculated from molecular field theory (___ $AFM\rho(\varepsilon_F)$ --- $PM\rho(\varepsilon_F)$).

Fig. 12b. Magnetic moment of Gd in Ni-Gd compounds as function of temperature calculated from molecular field theory (___ $AFM\rho(\varepsilon_F)$ --- $PM\rho(\varepsilon_F)$).

scaling of the induced moment by the magnitude of the localized Gd moment. The analogous results for the Ni alloys are shown on figs. 10, 11 and 12.

We might try to find a relation between the intra-atomic Coulomb interaction in the band theory and the exchange interaction of the quasi spins with the band electrons. It is known that (Liu 1976) conventional band theory cannot describe the paramagnetic properties of iron for example, because iron retain the local moment in the paramagnetic fase. Liu (1976) described the properties of itinerant magnetism by introducing a quasi spin model. It is also known that at low temperature the band description is sufficiently good. We assume that the quasi spin of iron has the same absolute value as at zero temperature but is precessing like a unit quasi spin (Liu 1976). From band theory in the Hartree Fock approximation we have that the band spliting is equal

$$\Delta = \epsilon_{i\downarrow} - \epsilon_{i\uparrow} = U(\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle) \tag{45}$$

where ϵ_{is} is defined previously (13).
For five fold degenerate bands we have (Hasegawa, Kanamori, 1972).

$$U = U_o + 4I, \tag{46}$$

where, U_o, is the intra-atomic Coulomb repulsion and, I, the interband exchange interaction. From the quasi spin model we have a band spliting equal

$$\Delta = 2jS \tag{47}$$

where S is the quasi spin and j the exchange integral between the quasi spin and the band electrons, determined from T_c(9). Only one band is considered and we expect j to be related to U_o. For low temperatures we have

$$S = \frac{5}{2}(\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle) \tag{48}$$

So we can formaly interprete (neglecting interband mixing) that $U_o(\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle)$ is comming from the interaction between the quasi spin and the band electrons. If we assume that j does not change very much with temperature we have the relation

$$j \cdot 2\,\frac{5}{2}(\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle) = U_o(\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle) \tag{49}$$

From that we find

$$j = \frac{U_o}{5} \tag{50}$$

Using the data of U and j (tables 1, 3) and relation (46) we can calculate interband interaction, I, given in table 4.

Metal	Co	Ni	Fe
I^{AFM} (eV)	0.4	0.2	0.5
I^{PM} (eV)	0.4	0.3	0.5

Table 4. Calculated interband exchange interaction, I.

These values are in agreement with those calculated by Hasegawa and Kanamori (Kanamori 1963, Hasegawa and Kanamori 1972) who obtained that I is ranging from 0.6 eV to 0.2 eV.

5. CONCLUSION

The conclusion we may draw is that the RKKY interaction between the localized R-spin and T-pseudo-spin mediated by an effective alloy medium well accounts for the magnetic moments and the transition temperatures. For low symmetry lattice structure, the CPA theory and elliptic density of states is a good approximation; for higher symmetry structures, a more realistic density of states as function of energy must be taken into account. Band structure calculations for these materials would be of interest in order to establish their densities of states and make possible a more detailed comparison with experiment.

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